

The chemistry and cell parameters of omphacites and related pyroxenes

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SUMMARY. In an attempt to correlate the chemical compositions and cell sizes of omphacites and related pyroxenes, the cell dimensions of fifty-five analysed pyroxenes have been determined, or taken from the literature. Twenty-two of the chemical analyses are new, nineteen of them being done by electron microprobe. Approximately two-thirds of the total number of analyses may be considered first class, the remainder are of doubtful or unknown quality. Cell parameters, determined by X-ray powder diffraction methods, have errors of $\pm 0.1\%$ for the majority of samples, although for some samples taken from the literature errors are unknown.

The majority of methods of recalculating omphacite analyses into their end-member molecules are unsuitable for correlation of cell constants with chemistry, mainly due to the impossibility of graphical representation of more than three end-member molecules, and to the non-stoichiometry of these molecules. Using a modification of Tröger's (1962) method of recalculating chloromelanite analyses the present analyses have been recalculated into the diopside-jadeite-acmite and diopside-jadeite-hedenbergite molecules and compared with their determined cell parameters. Because of the gradations in all parameters between these end-member molecules, determination of compositions based on the cell parameters (a , b , c , vol , or β) can only be made within wide limits. However, using a method of projection of compositions from the acmite and hedenbergite apices to the diopside-jadeite join the ratios of diopside to jadeite can be determined for most samples to within ± 5 mol %. As these are the most important constituents of most omphacites, this method permits an approximate estimation of omphacite compositions. From a knowledge of the cell sizes of the omphacite a rough indication of the conditions of formation of its host rock may also be obtained.

OMPHACITE is the principal pyroxene occurring in eclogitic rocks. The chemical complexity and difficulties frequently encountered in the separation of omphacites from their host rocks make analysis of this mineral by standard wet chemical techniques tedious and complex. Although the use of the electron microprobe eliminates to some degree problems of separation, the lack of suitable standards and the inability of the microprobe to determine Fe^{2+} and Fe^{3+} make analysis of omphacites far from routine. Nevertheless, the compositions of omphacites are important indicators of the mode of formation of eclogites (cf. Eskola, 1921; Coleman *et al.*, 1965; Smulikowski, 1965) and it is desirable that some rapid method, based on an easily determined physical property, be available to determine the composition of the pyroxenes in these rocks. The most obvious choices of physical properties are optical and X-ray parameters, both requiring a minimum amount of material and separation. Previous attempts to correlate compositions of omphacites are those of Tröger (1951) based on optical properties; Essene and Fyfe (1967), based on combined optical and X-ray data; and Seki and Onuki (1967), based on X-ray data. However, although these studies indicate that the compositions of omphacites can be determined by

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physical methods, they are based either on very few samples or on samples from only one area.

In an attempt to develop a new method, based on comparison of composition with cell parameters determined by X-ray powder diffraction methods, the cell constants of fifty-five analysed omphacites and related pyroxenes (principally containing diopside and jadeite) have been determined. Twenty-two of the analyses are new, of which nineteen have been determined on the MAC-400 electron microprobe. The remaining analyses have been taken from the literature, as well as a few of the cell parameters. Approximately two-thirds of the data may be considered first-class, the remainder being of doubtful or unknown quality. Samples, geographical location, rock type, and donors are listed in table I, chemical analyses are presented in table II.

Chemical and X-ray methods. For the majority of samples, not supplied in a purified state, preliminary separation was done by isodynamic separator and heavy liquids with final purification by hand-picking from the 60 to 100 mesh fractions. For samples requiring chemical analysis about 2 g of purified material was required while for samples already analysed only 50–60 mg was required. Purity of the sample was checked optically and by X-ray diffraction methods. For most samples purity was about 99 % although in a few cases amphibole peaks were detected in the X-ray patterns indicating a lower degree of purity. The recalculated analyses in table II indicate high purity for most samples analysed.

Analyses were done in duplicate by standard wet chemical (Peck, 1964) and photometric techniques (Shapiro and Brannock, 1962). Electron microprobe analysis were done on an MAC-400 microprobe using a spot size of 2 μ at 15 kV and 0.01 μ amps, reading the $K\alpha$ lines, and using the off-peak background method. Due to lack of any known standards for omphacitic pyroxenes, the sample from the Roberts–Victor Mine (no. 33) and from Silberbach (no. 4) were taken as standards. The analyses of both of these samples were believed to be of high quality. For all samples analysed by the microprobe, FeO and Fe₂O₃ were determined by wet chemical methods.

Cell parameters, given in table III, were determined from powdered material using Si as an internal standard and run on a Norelco high-angle diffractometer. Patterns were indexed using the spacings of Warner (1964) and Yoder (1950), with 12 to 15 planes being measured for each sample. Parameters were computed using a least-squares programme written by Mozzi and Newell (1961). The magnitudes of the errors are also given in table III. In the few samples where parameters obtained in the present study could be compared with those obtained by other investigators, the comparison was very close, as shown in table IV.

Results. The chemical analyses of all of the pyroxenes used in this study are given in table II and the most probable origin for the host eclogite, according to Smulikowski's (1964) classification, is also listed. Eleven samples are from Group I (ultrabasic garnet–pyroxene rocks), twenty-seven from Group II (ophiolitic eclogites), fourteen from Group III (eclogites in gneiss and migmatite complexes), and two whose group is unknown.

The cell parameters listed in table III show a wide range; for the majority of samples the errors are low. For the few samples taken from the literature errors are unknown. Samples determined in the present study with large errors are caused either by interference from planes of other minerals that could not be removed during separation or by poor peak resolution; both factors result in a small number of planes being used in the final computation of the parameters.

Although numerous methods have been proposed for the recalculation of omphacites into their many possible 'end-member' molecules, for reasons discussed below, only the method of Tröger (1962) is suitable for the present study.¹ This method as modified is outlined in the Appendix and the results of the recalculations are shown in table V.

Discussion of results. The principal end-members of omphacites are diopside, jadeite, acmite, hedenbergite, orthopyroxenes, wollastonite, and various Tschermak's molecules. Although many investigators have devised methods to plot the complex composition of this pyroxene (cf. Eskola, 1921; Tröger, 1962; Kushiro, 1962; Yoder and Tilley, 1962; White, 1964; Coleman *et al.*, 1965; Huckenholz, 1965; Smulikowski, 1965; Vogel, 1966; Church, 1968a), the majority of these methods are unsuitable, for one reason or another, when used to compare the chemistry and cell parameters of omphacites. Without exception these methods have been used to distinguish the different chemistry of various pyroxenes and not to correlate their compositions with any physical property.

In order to make a useful correlation between cell parameters and chemistry of any complex solid-solution series the following conditions must be fulfilled:

The composition of the mineral must be representable in terms of not more than three end-member molecules in order that it can be plotted on a two-dimensional (i.e. planar) surface.

The end-member molecules must be stoichiometric (i.e. $\text{CaMgSi}_2\text{O}_6$, not $\text{Ca}(\text{Mg,Fe})\text{Si}_2\text{O}_6$) and have good cell constants, preferably from synthetic material.

The cell constants of the end-members chosen should be sufficiently different to provide the greatest possible accuracy. All of the end members should belong to the same crystal system.

On the assumption of complete, or even partial, solid solution between each of the end-member molecules, the different parameters should fall in different 'directions' when plotted on a triangular or other geometric figure. For example if there are three end-members, all monoclinic, when plotted on a triangular diagram the four parameters (a , b , c , β) should lie in different directions. This is illustrated with reference to fig. 1 (p. 69). Assume three end-member molecules A, B, and C, with complete solid solution between A-B, B-C, and A-C and possible solid solution between A, B, and C, then, according to Vegard's Law, there should be a linear gradation between any of the cell constants of one end-member with the addition of a second end-member. Thus, if lines are drawn on the diagram representing constant expected parameters (these may be termed 'isoparameter lines') the ideal situation for comparison of composition with chemistry is shown in figs. 1a-c where these lines are in different directions. In fig. 1d the three parameters have been superimposed, producing a grid of isoparameters. Obviously the more parameters obtained, the greater will be the refinement of the grid. Thus by determining the parameters and plotting them on such a grid it is possible

¹ A modification of the method of White (1964) to recalculate omphacites in terms of Ca-Tschermak-diopside-jadeite end-members fulfills the stipulated conditions as discussed below but gave very poor results possibly indicating that the Ca-Tschermak molecule is not as important as the acmite or hedenbergite.

TABLE I

No.	Locality	Rock association	Group†	Reference on the area	Donor (or source of reference)	Original number
<i>First-class data (wet chemical analyses)</i>						
1	Kupplerbrunn, Saualpe, Austria	amphibolitic eclogite	III	Mottana <i>et al.</i> (1968)	W. R. Church	{3b
2	Burgstein, Oetzal, Austria	amphibolitic eclogite	I	Hezner (1903)		{O-1
3	Ballyshannon, Donegal Co., Eire	plagioclase eclogite	III	Church (1968 <i>a</i>)		{6c
4	Silberbach, Bavaria, Germany	zoisite eclogite	III	Yoder & Tilley (1962)	E. J. Essene	C.958
5	Leverburgh, S. Harris, Scotland	amph-opx eclogite	III	Livingstone (1967)	A. Livingstone	B.10
6	Lyell Highway, Tasmania	amph-mica eclogite	III	Spry (1963)	A. Spry	—
7	Junction School, California	eclogite	II	Coleman <i>et al.</i> (1965)	E. D. Jackson	{102-RGC-59
8	Valley Ford, California	mica eclogite	II	Switzer (1945)	E. J. Essene	{207-RGC-58
9	Healdsburg, California	vein in glauc. schist	II	Wolfe (1955)	—	{H.6
10	Cloverdale, California	eclogite	II	Coleman <i>et al.</i> (1965)	Clarke & Papike (1968)	{100-RGC-58
11	Tiburon pen., California	vein in serpentinite	II	Coleman (1961)	Coleman & Clark (1968)	{R-1854
12	Clear Creek, California	green pod-like body	I?	Schmitt (1963)	—	{R-1853
13	Eiksundsdal, Sunmøre, Norway	hypersthene eclogite	III	Kappel (1967)	J. Warner (1964)	1725
14	Mitterbachgraben, Lower Austria	plagioclase eclogite	I	Foshag (1955)	F. Kappel (1967)	—
15	Kaminaljuyu, Guatemala	tomb	?	McBirney <i>et al.</i> (1967)	Clark & Papike (1968)	2
16	Manzanal, Guatemala	albite-jadefite boulder	II	Coleman <i>et al.</i> (1965)	McBirney <i>et al.</i> (1967)	—
17	Amos Stream, New Caledonia	amph-mica eclogite	II	—	Clark & Papike (1968)	36-NC-62
<i>First-class data (microprobe analyses)</i>						
19	Burlington pen., Newfoundland	amphibolitic eclogite	III	Church (1968 <i>b</i>)	W. R. Church	A.1
20	Biella, Piemonte, Italy	qz-omph-fels	II	Bianchi & Dal Piaz (1963)	W. R. Church	M.1
21	Lago Mucrone, Piemonte, Italy	glaucoph-eclogite	II?	—	P. Bearth	PVB 670
22	Quincetto, Piemonte, Italy	omphacite	II?	—	A. Boriani	—
23*	(Val Pellice?), Piemonte, Italy	retrograded eclogite	II	Smulikowski (1964)	collections	{PVB 644
24	Nowa Wies, Sudetes, Poland	amphibolitic eclogite	III	Bearth (1965)	P. Bearth	{PB 1305
25	Mellichen, Wallis, Switzerland	metagabbro	III	Vogel (1966)	—	{CO 6A
26	Cabo Ortegal, Galicia, Spain	zoisite eclogite	III	Lacroix (1917)	W. R. Church	{LC-L
27	Lherz, Ariège, France	garnet {light fract.}	I	—	—	{LC-H
28	—	ariegite {heavy fract.}	I	—	—	—

OMPHACITES

29	(Silberbach?), Bavaria, Germany		III	Chesnokov-Popov (1965)	W. Griffin	—
30	Salt Lake Crater, Oahu, Hawaii	qz-musc-eclogite	I	Yoder & Tilley (1962)	E. D. Jackson	67-SAL-1
31	Bultfontein mine, S. Africa	gar-cpx-(opx) nodule	I	Jackson (1966)	W. Griffin	{ KA-64-5
32	Roberts-Victor Mine, S. Africa	eclogite nodule	I	Williams (1932)	collections	{ KA-64-6
33	Valley Ford, California	eclogite nodule	I	Bloxam (1959)	A. Nicolas	{ VF 1
34	Uja di Ciarnarella, Piemonte, Italy	muscovite eclogite	II	Nicolas (1966)		{ VF 2
35		musc.-glauc. eclogite	II			515
36		glauc.-eclogitic schist	II			
<i>Second-class data (wet chemical analyses)</i>						
37	Pian Comune, Piemonte, Italy	eclogitic gabbro	II	Nicolas (1966)	A. Nicolas	{ 484
38*	Ala di Stura, Piemonte, Italy	metagabbro	II			{ 479
39	Stura di Viù, Piemonte, Italy	vein in diabase	II?	Hashimoto (1964)	recalc. powder pattern	{ 369A
40	Asahine, Kanto Mts., Japan	albite jadeite dike	?	Lacroix (1930)	E. J. Essene	—
41	Tawmaw, Kachin Hills, Burma	eclogite	II	Ginzburg & Sidorenko (1964)	rec. from KX to Å	5618
42	Khalikovo, Urals, U.S.S.R.		II			—
43	Fay-de-Bretagne, L.-A., France	paragon, { fract. A fract. B fract. L fract. H ecl.	III	Velde (1966)	Velde (1966) recalc. from published powder patterns	—
44		biminerale eclog.	I	Kappel (1967)	recalc. powder pattern	—
45	Meidling im Tal, Lower Austria	—	II	—	Clark & Papike (1968)	2833
46	Guajira pen., Colombia	muscovite eclogite	II	McBirney <i>et al.</i> (1967)	McBirney <i>et al.</i> (1967)	G-724
47	El Rosario, Guatemala	omphacite fels	II	Bearth (1965)	P. Bearth	PB-1320
48*	Findelen, Wallis, Switzerland	ecl. incl. in dunite	I	Miyashiro & Seki (1958)	Seki & Onuki (1968)	—
49	Gongen-yama, Sikoku, Japan	metabasalt	II	Coleman <i>et al.</i> (1965)	Coleman & Clark (1968)	15-CZ-60
50*	Ward Creek, California		II			—
<i>Second-class data (microprobe analyses)</i>						
51	Val Germanasca, Piemonte, Italy	eclogite	II	—	collections	—
52	Mt. Boardman, California	vein in glauc. schist	II	Essene & Fyfe (1967)	E. J. Essene	{ 88-5M-2
53	S. Berkeley Hills, California	gar-cpx rock	II			{ M-541

* In sample 23 there are two coexisting pyroxenes (white and green). Analysis and X-ray data refer to the green fraction. Sample 38 is extremely inhomogeneous and may be a mixture of many pyroxenes in disequilibrium. Sample 50 shows irregular patches of diopside-rich and jadeite-rich pyroxenes within the same grain under the microprobe. Of sample 48 no full analysis has been published but only the formula.

† After Smulikowski (1964).

TABLE II. *New chemical analyses of omphacites, with atomic ratios to six oxygen*

	1	2	3	19	20	21	22	23	24	25	26
SiO ₂	54.08	54.53	51.25	56.3	58.0	57.1	57.7	57.7	56.5	57.7	55.0
TiO ₂	0.14	0.02	0.38	—	—	—	—	—	—	—	—
Al ₂ O ₃	9.20	8.91	4.86	10.2	12.9	13.3	14.7	6.4	11.3	12.5	10.9
Fe ₂ O ₃	0.83	0.96	2.21	2.0	1.0	0.9	1.1	1.3	0.1	0.7	1.5
FeO	2.18	2.06	6.36	2.2	1.8	1.4	1.7	1.2	2.4	2.5	2.7
MnO	tr.	0.03	0.08	—	—	—	—	—	—	—	—
MgO	11.51	11.43	12.54	9.6	7.8	8.0	6.9	12.1	9.8	7.3	9.9
CaO	17.50	17.48	20.89	15.0	12.5	13.6	12.2	17.7	15.3	13.9	15.8
Na ₂ O	4.20	4.36	1.50	5.6	6.1	7.0	7.3	3.7	5.5	7.0	4.3
K ₂ O	0.04	0.03	0.06	—	—	—	—	—	—	—	—
H ₂ O+	0.46	0.26	—	—	—	—	—	—	—	—	—
	100.14	100.07	100.13	100.9	100.1	101.3	101.6	100.1	100.9	101.1	100.1
Si	1.938	1.951	1.897	1.98	2.02	1.98	1.98	2.04	1.98	2.01	1.95
Al ^{iv}	0.062	0.049	0.103	0.02	—	0.02	0.02	—	0.02	—	0.05
Al ^{vi}	0.327	0.327	0.109	0.40	0.53	0.52	0.57	0.27	0.45	0.51	0.41
Ti	0.004	0.000	0.011	—	—	—	—	—	—	—	—
Fe ³⁺	0.002	0.026	0.062	0.05	0.03	0.02	0.03	0.03	0.01	0.02	0.04
Fe ²⁺	0.065	0.062	0.197	0.07	0.05	0.04	0.05	0.04	0.07	0.06	0.08
Mn	0.000	0.000	0.003	—	—	—	—	—	—	—	—
Mg	0.615	0.609	0.692	0.50	0.40	0.41	0.35	0.64	0.51	0.38	0.52
Ca	0.675	0.671	0.828	0.56	0.47	0.51	0.45	0.67	0.57	0.52	0.60
Na	0.292	0.305	0.108	0.38	0.41	0.47	0.49	0.26	0.37	0.47	0.30
K	0.002	0.001	0.003	—	—	—	—	—	—	—	—
Σ cat.	4.002	4.001	4.013	3.96	3.91	3.97	3.94	3.95	3.98	3.97	3.95
	27	28	29	30	31	32	33	34	35	36	53
SiO ₂	53.6	54.1	57.0	50.1	50.3	52.7	56.47	57.7	57.4	57.4	55.7
TiO ₂	—	—	—	—	0.5	—	—	—	—	—	—
Al ₂ O ₃	7.4	3.8	8.2	9.0	9.4	9.6	7.14	9.4	11.9	12.0	8.1
Fe ₂ O ₃	0.4	0.4	0.6	2.5	1.6	3.1	2.4	2.5	4.6	3.3	3.1
FeO	2.6	2.6	0.7	4.6	3.8	3.2	3.6	2.4	2.2	4.0	4.4
MnO	—	—	—	—	—	—	—	—	—	—	—
MgO	13.4	13.0	12.1	11.3	12.5	10.0	11.89	8.5	6.5	6.0	7.5
CaO	21.0	24.4	18.1	18.0	19.4	20.2	13.76	12.0	11.8	11.0	13.9
Na ₂ O	1.3	1.1	3.1	2.9	2.4	2.7	4.95	7.8	7.1	7.1	6.2
K ₂ O	—	—	—	—	—	—	0.13	—	—	—	—
H ₂ O+	—	—	—	—	—	—	—	—	—	—	—
	99.7	99.4	99.8	98.4	99.9	100.9	100.47	100.3	101.5	100.8	98.9
Si	1.93	1.98	2.01	1.86	1.93	1.89	2.007	2.03	2.00	2.02	2.03
Al ^{iv}	0.07	0.02	—	0.14	0.07	0.11	—	—	—	—	—
Al ^{vi}	0.25	0.14	0.34	0.25	0.35	0.29	0.299	0.39	0.49	0.50	0.35
Ti	—	—	—	—	0.01	—	—	—	—	—	—
Fe ³⁺	0.01	0.01	0.01	0.07	0.05	0.08	0.064	0.07	0.12	0.09	0.09
Fe ²⁺	0.08	0.08	0.12	0.14	0.12	0.10	0.107	0.07	0.06	0.12	0.13
Mn	—	—	—	—	—	—	—	—	—	—	—
Mg	0.72	0.71	0.64	0.62	0.41	0.53	0.630	0.45	0.34	0.31	0.41
Ca	0.81	0.95	0.68	0.72	0.80	0.77	0.524	0.46	0.44	0.41	0.54
Na	0.09	0.08	0.21	0.21	0.18	0.19	0.341	0.54	0.48	0.48	0.44
K	—	—	—	—	—	—	0.006	—	—	—	—
Σ cat.	3.96	3.97	3.91	4.01	3.92	3.96	3.982	4.01	3.93	3.93	3.99

1 and 2. Anal. A. Mottana (wet chemical analyses).

3. Anal. O. Von Knorring (wet chemical analysis).

33. Anal. P. Ribbe (microprobe analysis: includes 0.13 % Cr₂O₃).

19 to 53. Anal. N. D. MacRae (microprobe analyses).

In all microprobe analyses the iron has been distributed between Fe₂O₃ and FeO on the basis of semi-chemical quantitative analysis of FeO by A. Mottana.

— not determined.

TABLE III. Cell parameters of pyroxenes

No.	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	β	<i>V</i> (Å ³)
1	9.671 ± 0.009	8.842 ± 0.009	5.212 ± 0.005	106.77 ± 0.08	426.7 ± 1.1
2	9.621 ± 0.008	8.807 ± 0.007	5.265 ± 0.004	106.59 ± 0.01	427.6 ± 0.9
3	9.671 ± 0.007	8.885 ± 0.006	5.237 ± 0.004	107.01 ± 0.05	430.3 ± 0.8
4	9.662 ± 0.004	8.845 ± 0.004	5.248 ± 0.002	106.37 ± 0.02	430.3 ± 0.6
5	9.725 ± 0.004	8.902 ± 0.004	5.251 ± 0.002	106.09 ± 0.02	436.3 ± 1.1
6	9.652 ± 0.006	8.830 ± 0.006	5.230 ± 0.003	106.36 ± 0.03	427.7 ± 0.8
7	9.582 ± 0.009	8.789 ± 0.008	5.226 ± 0.005	106.95 ± 0.03	421.0 ± 1.2
8	9.606 ± 0.007	8.796 ± 0.006	5.274 ± 0.004	106.83 ± 0.04	426.5 ± 0.7
9	9.667 ± 0.008	8.794 ± 0.007	5.216 ± 0.004	106.78 ± 0.04	424.5 ± 1.1
10	9.451 ± 0.005	8.614 ± 0.005	5.249 ± 0.003	107.50 ± 0.03	407.5 ± 0.8
11*	9.596 ± 0.005	8.771 ± 0.004	5.265 ± 0.006	106.93 ± 0.05	423.9 ± 0.4
12*	9.437 ± 0.006	8.574 ± 0.006	5.225 ± 0.006	107.58 ± 0.08	403.0 ± 1.0
13*	9.486 ± 0.008	8.622 ± 0.006	5.241 ± 0.004	107.58 ± 0.08	408.6 ± 1.1
14*	9.662 ± 0.003	8.819 ± 0.004	5.228 ± 0.002	106.55 ± 0.02	427.0 ± 0.5
15*	9.7264 ± n.d.	8.8328 ± n.d.	5.2546 ± n.d.	106.18 ± n.d.	433.6 ± n.d.
16*	9.559 ± 0.006	8.762 ± 0.006	5.245 ± 0.006	106.92 ± 0.07	420.3 ± 0.4
17*	9.439 ± 0.001	8.5846 ± 0.0004	5.226 ± 0.002	107.46 ± 0.02	404.0 ± 0.2
18*	9.595 ± 0.006	8.786 ± 0.009	5.260 ± 0.006	106.87 ± 0.10	424.4 ± 0.6
19	9.620 ± 0.004	8.805 ± 0.003	5.253 ± 0.002	106.68 ± 0.01	426.2 ± 0.4
20	9.552 ± 0.009	8.780 ± 0.008	5.209 ± 0.005	106.59 ± 0.05	418.7 ± 1.1
21	9.569 ± 0.006	8.766 ± 0.006	5.249 ± 0.003	106.90 ± 0.02	421.3 ± 0.8
22	9.546 ± 0.007	8.751 ± 0.006	5.230 ± 0.004	106.90 ± 0.02	419.7 ± 0.9
23	9.686 ± 0.009	8.852 ± 0.008	5.239 ± 0.005	106.25 ± 0.04	431.2 ± 1.3
24	9.618 ± 0.009	8.809 ± 0.008	5.221 ± 0.005	106.78 ± 0.05	423.8 ± 0.7
25	9.604 ± 0.005	8.793 ± 0.005	5.205 ± 0.003	106.80 ± 0.02	420.8 ± 0.5
26	9.640 ± 0.008	8.815 ± 0.007	5.229 ± 0.004	106.32 ± 0.04	426.4 ± 1.2
27	9.695 ± 0.009	8.921 ± 0.008	5.227 ± 0.005	106.78 ± 0.03	432.9 ± 1.2
28	9.715 ± 0.005	8.881 ± 0.005	5.245 ± 0.003	106.11 ± 0.03	434.8 ± 0.8
29	9.660 ± 0.007	8.844 ± 0.006	5.228 ± 0.004	106.31 ± 0.04	428.4 ± 1.3
30	9.707 ± 0.004	8.847 ± 0.004	5.287 ± 0.002	106.62 ± 0.02	435.1 ± 0.5
31	9.718 ± 0.008	8.878 ± 0.007	5.240 ± 0.004	106.35 ± 0.03	433.8 ± 1.0
32	9.692 ± 0.006	8.856 ± 0.005	5.240 ± 0.003	106.22 ± 0.03	431.8 ± 0.9
33	9.663 ± 0.006	8.809 ± 0.005	5.246 ± 0.003	106.92 ± 0.02	427.2 ± 0.8
34	9.609 ± 0.005	8.788 ± 0.004	5.262 ± 0.003	106.84 ± 0.04	425.5 ± 0.5
35	9.597 ± 0.009	8.796 ± 0.008	5.247 ± 0.005	106.85 ± 0.04	423.9 ± 1.3
36	9.582 ± 0.013	8.774 ± 0.012	5.213 ± 0.007	106.92 ± 0.06	419.3 ± 1.5
37	9.618 ± 0.009	8.788 ± 0.008	5.219 ± 0.005	106.71 ± 0.05	422.5 ± 1.1
38	9.662 ± 0.004	8.829 ± 0.004	5.204 ± 0.002	106.60 ± 0.02	525.2 ± 0.6
39	9.428 ± 0.005	8.566 ± 0.005	5.239 ± 0.003	107.72 ± 0.04	403.0 ± 0.6
40	9.601 ± 0.006	8.774 ± 0.006	5.269 ± 0.003	106.96 ± 0.05	424.5 ± 0.9
41	9.48 ± 0.02	8.63 ± 0.02	5.18 ± 0.01	107.3 ± 0.1	404.6 ± 2.8
42*	9.45 ± n.d.	8.82 ± n.d.	5.16 ± n.d.	106.6 ± n.d.	412.0 ± n.d.
43	9.609 ± 0.007	8.796 ± 0.006	5.245 ± 0.004	106.67 ± 0.02	425.2 ± 0.3
44	9.623 ± 0.006	8.806 ± 0.006	5.215 ± 0.003	106.49 ± 0.03	423.8 ± 0.6
45	9.617 ± 0.010	8.800 ± 0.009	5.254 ± 0.006	106.74 ± 0.03	425.8 ± 1.3
46	9.604 ± 0.009	8.791 ± 0.008	5.247 ± 0.005	106.65 ± 0.03	424.4 ± 1.1
47	9.723 ± 0.011	8.842 ± 0.010	5.277 ± 0.006	106.39 ± 0.03	435.2 ± 1.6
48	9.596 ± 0.005	8.786 ± 0.004	5.267 ± 0.006	106.92 ± 0.07	424.4 ± 0.4
49*	9.56 ± 0.01	8.78 ± 0.01	5.25 ± 0.01	106.78 ± 0.08	421.6 ± 2.2
50	9.585 ± 0.005	8.772 ± 0.004	5.256 ± 0.003	106.94 ± 0.01	422.7 ± 0.8
51*	9.75 ± n.d.	8.93 ± n.d.	5.25 ± n.d.	105.80 ± n.d.	439.8 ± n.d.
52*	9.58 ± 0.02	8.75 ± 0.02	5.36 ± 0.05	107.02 ± 0.17	429.7 ± 7.8
53	9.63 ± 0.03	8.81 ± 0.03	5.25 ± 0.02	106.4 ± 0.1	427.3 ± 4.6
54	9.62 ± 0.02	8.78 ± 0.02	5.31 ± 0.01	108.6 ± 0.1	425.1 ± 2.9
55	9.75 ± 0.01	8.79 ± 0.01	5.19 ± 0.01	106.9 ± 0.1	425.6 ± 1.9

* Data taken from literature (see table I for reference).

n.d. not determined.

TABLE IV. Comparison between cell parameters determined and taken from the literature

No.	<i>a</i>	<i>b</i>	<i>c</i>	β	Reference
5	$9.725 \pm 0.004 \text{ \AA}$	$8.902 \pm 0.004 \text{ \AA}$	$5.251 \pm 0.002 \text{ \AA}$	$106.09^\circ \pm 0.02$	Present study. A. Livingstone (personal communication)
	9.714	8.881	5.250	106.12	
10	9.451 ± 0.005	8.614 ± 0.005	5.249 ± 0.003	107.50 ± 0.003	Present study. (H.S.Yoder in Wolfe, 1955; Wolfe, 1955)*
	9.45	8.57	5.25		
	9.48	8.59	5.23	107.42	
13	9.506 ± 0.012	8.636 ± 0.011	5.249 ± 0.007	107.57 ± 0.08	†
	9.486 ± 0.008	8.622 ± 0.006	5.241 ± 0.004	107.58 ± 0.08	
15	9.683 ± 0.013	8.858 ± 0.012	5.239 ± 0.007	106.15 ± 0.04	Coleman & Clark (1968)
	9.7264	8.8328	5.2546	106.18	
40	9.601 ± 0.006	8.774 ± 0.006	5.269 ± 0.003	106.96 ± 0.05	Kappel (1967)
	9.60	8.77	5.27	106.90	
					Present study. Seki & Onuki (1967)

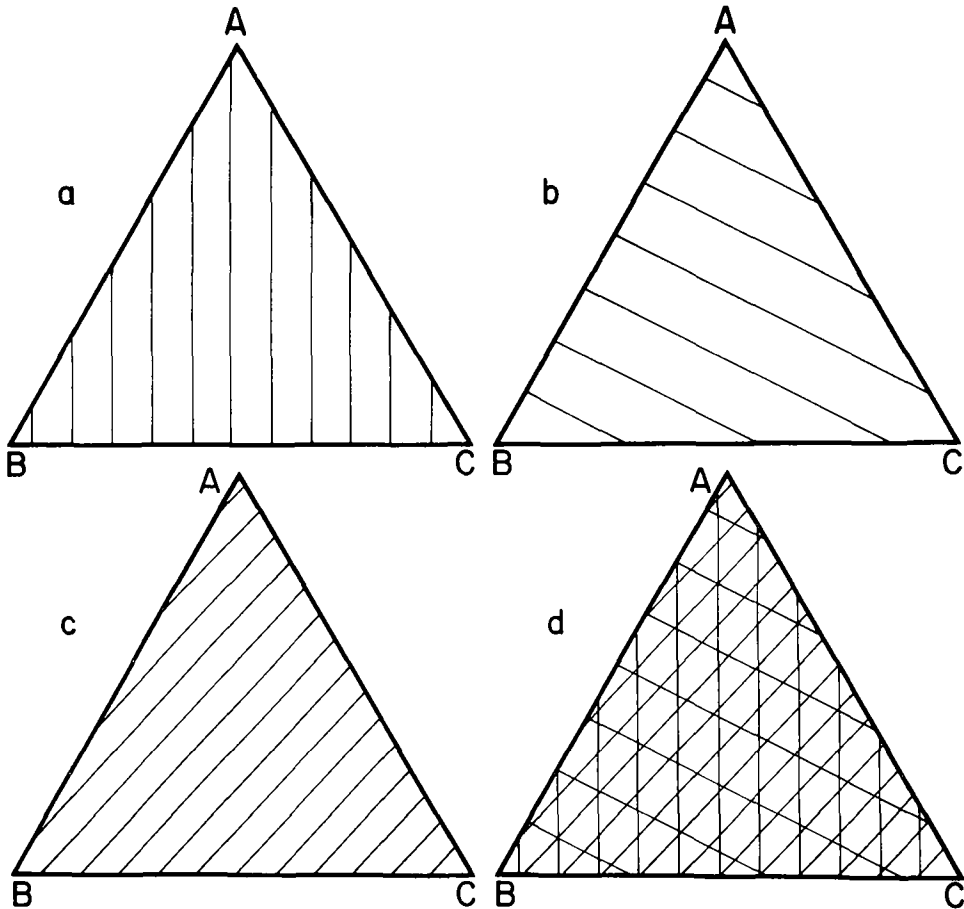
* Determined by single crystal method (all the other determinations by powder techniques).

† Computed from published powder pattern but not referred in table II in preference to that of the literature source.

TABLE V. Recalculated end members of pyroxenes

No.	Ac	Jd	Di	Jd	Di	Hd	No.	Ac	Jd	Di	Jd	Di	Hd
1	2.5	29.7	67.8	28.6	65.2	6.2	29	1.1	23.5	75.4	23.2	74.5	2.3
2	3.2	33.9	62.9	32.4	60.1	7.4	30	8.5	16.8	74.7	16.2	72.0	11.7
3	7.6	7.3	85.1	6.6	77.7	15.7	31	8.4	22.0	69.5	19.7	62.1	18.2
4	0.5	24.6	74.9	23.7	72.2	4.1	32	11.1	15.3	73.6	14.9	71.6	13.5
5	3.1	11.1	85.8	9.9	76.6	13.5	33	5.1	34.4	60.5	—	—	—
6	6.2	35.2	58.6	33.6	56.1	10.3	34	7.1	47.5	45.4	50.6	48.3	1.1
7	13.0	40.4	46.6	41.4	47.9	10.7	35	14.6	43.9	41.5	47.4	44.8	7.8
8	17.4	36.3	46.3	38.9	49.8	11.3	36	11.4	49.4	39.2	48.7	38.7	12.6
9	12.4	36.5	51.1	36.5	52.5	10.0	37	5.4	37.8	48.9	—	—	—
10	0.9	93.5	5.6	94.3	5.7	0.0	38	6.0	29.6	64.4	29.0	62.9	8.1
11	10.8	41.3	47.9	42.7	49.4	7.9	39	2.2	92.0	5.8	92.4	5.8	1.8
12	1.0	98.2	0.8	98.8	0.8	0.4	40	13.3	40.3	46.4	41.1	47.3	11.5
13	15.3	77.1	7.6	88.0	8.7	3.3	41	4.0	93.0	3.0	—	—	—
14	13.8	22.0	64.2	26.4	73.3	0.3	42	19.8	33.4	46.8	41.6	58.4	0.0
15	4.5	12.0	83.5	12.1	84.2	3.7	43	6.6	32.8	60.6	32.9	60.8	6.3
16	2.3	48.2	49.5	49.3	50.5	0.2	44	4.6	34.3	61.1	34.0	60.7	5.3
17	0.8	94.2	5.0	94.8	5.0	0.2	45	2.6	37.9	59.5	36.5	58.3	5.2
18	12.0	41.0	47.0	40.7	46.7	12.6	46	4.3	34.8	60.9	34.7	60.6	4.6
19	6.8	35.9	57.3	36.0	57.4	6.6	47	1.8	11.6	86.6	—	—	—
20	3.7	46.9	49.4	45.8	48.2	6.1	48	7.8	42.5	49.7	41.1	48.2	10.7
21	2.3	51.1	46.6	50.0	45.6	4.4	49	6.6	42.2	51.2	42.5	51.7	5.8
22	3.6	54.8	41.6	53.6	40.7	5.8	50	8.7	45.7	45.6	47.1	47.1	5.8
23	3.3	25.6	71.1	25.6	71.1	3.3	51	0.5	0.0	99.5	0.0	97.1	2.9
24	1.2	40.9	57.9	38.7	54.8	6.5	52	7.6	44.8	47.6	42.4	45.1	12.5
25	2.3	53.0	44.7	50.5	42.6	6.8	53	10.6	41.2	48.2	39.4	46.1	14.6
26	4.8	31.7	63.5	30.3	60.5	9.2	54	48.2	47.0	4.9	—	—	—
27	1.2	8.7	90.1	8.0	82.8	9.2	55	9.8	1.2	88.9	1.0	71.9	27.1
28	1.2	8.7	90.1	8.0	83.0	9.0							

to 'pigeon-hole' the composition of the mineral. If the parameters all fall in the same or similar directions such a grid will not delineate a small area of the geometric figure and be of little use for the present purposes. For setting up such a system it is not necessary that there be complete solid solution between the three end-members since



Figs. 1a-d. Lines of equal parameter plotted on triangular diagram representing three components.

compositions would not be expected to plot in areas in which there was no solid solution (provided, of course, the mineral had been as cleanly separated as possible).

These conditions may now be considered in the case of omphacites. Most of the samples used in this study have compositions that, when recalculated by almost any method, contain over 80 % of the diopside, jadeite, acmite, and hedenbergite molecules. Using the method of Tröger (1962), compositions can be recalculated as diopside-jadeite-acmite or as diopside-jadeite-hedenbergite. Most of their constituents can thus be graphically represented on a triangular diagram, fulfilling the first

condition. Tröger's (1962) method as modified also recalculates these molecules in their stoichiometric forms, for which there are good cell parameter data available from synthetic material: diopside, Clark *et al.*, 1962; jadeite, Frondel and Klein, 1965; acmite, Gilbert, 1966; and hedenbergite, Dr. J. Nolan, personal communication. From table VI it is clear that there is a large variation particularly in the *a* and *b* parameters in all of these minerals. Therefore, the second and third stipulated conditions are also fulfilled.

TABLE VI. Cell parameters of end-member molecules of pyroxenes

Mineral	<i>a</i> Å	<i>b</i> Å	<i>c</i> Å	β	V	Reference
Diopside	9.745 ± 0.001	8.925 ± 0.001	5.248 ± 0.001	105.87 ± 0.01	439.08 ± 0.07	Clark <i>et al.</i> (1962)
Jadeite	9.418 ± 0.006	8.563 ± 0.004	5.211 ± 0.006	107.57 ± 0.05	400.7 ± 0.6	Frondel & Klein (1965)
Acmite	9.660 ± 0.005	8.804 ± 0.005	5.289 ± 0.005	107.33 ± 0.05	429.4 ± 0.3	Gilbert (1966)
Hedenbergite	9.841 ± 0.005	9.027 ± 0.003	5.247 ± 0.003	104.80 ± n.d.	450.69 ± n.d.	Nolan (personal communication)

Examination of the parameters given in table VI show that the fourth condition is not fulfilled. Diopside and jadeite are the most important constituents of omphacites, acmite and hedenbergite being of only minor importance. Consideration of the *a* and *b* parameters of diopside, acmite, and jadeite show that they both decrease in that order. Thus when plotted on a triangular diagram the isoparameters all have approximately the same direction. The *c* parameter does not have this tendency but the differences between this parameter (5.294 Å for acmite to 5.211 Å for jadeite) are not sufficiently great. Similar problems are encountered with the diopside, jadeite, hedenbergite trio.

The criterion of complete or partial solid solution between the end-member molecules diopside, jadeite, acmite, and hedenbergite is probably fulfilled. Yagi (1958) has shown that there is complete solid solution in the diopside–acmite system at atmospheric pressure; diopside–jadeite shows partial solid solution at 30 kb with a miscibility gap between Di_{28} and Di_{90} (Bell and Davis, 1965); jadeite–acmite shows complete solid solution at 40 kb in the range Jd_{100} to Jd_{40} (mol %) (Gilbert, 1967). The range of solid solution of hedenbergite with the addition of jadeite and diopside is unknown, as is the range of ternary solid solutions in the diopside–jadeite–acmite and diopside–jadeite–hedenbergite systems.

Before considering the correlation of the chemistry and cell parameters of the pyroxenes of this study using Tröger's (1962) modification a brief explanation should be made concerning the inapplicability of the other methods. The methods of Eskola (1921) and Yoder and Tilley (1962) recalculate analysis in terms of more than three end-member molecules and in most cases these recalculations do not produce stoichiometric end-members. The latter reason also makes Church's (1968*a*) method inapplicable. In both Church's (1968*a*) and Smulikowski's (1965) method only 40 to 60 % of the determined cations are used in the recalculation. Kushiro's (1962) and Vogel's (1966) methods give errors for K and Ti since these cations when recalculated do not correspond to possible end-member molecules but probably to analytical errors. In Huckenholz's (1965) method, jadeite, hedenbergite, and acmite are added to diopside and when analyses are plotted they fall in a very narrow range of the diagram.

As mentioned previously, omphacites normally contain less than 10 wt % of acmite or hedenbergite when recalculated into either diopside–jadeite–acmite or diopside–jadeite–hedenbergite sets of end-members. Thus their parameters are mainly influenced by those of the diopside and jadeite molecules. On figs. 2 *a* and *b* the observed *b* parameters of all pyroxenes have been compared with the theoretical parameters when recalculated by Tröger's method into the diopside–jadeite–acmite and diopside–jadeite–hedenbergite end-members. Agreement between the observed and theoretical parameters is good. Similar agreement is found between the *a*, *a* sin β , and volume but there is very poor agreement between the *c* theoretical and

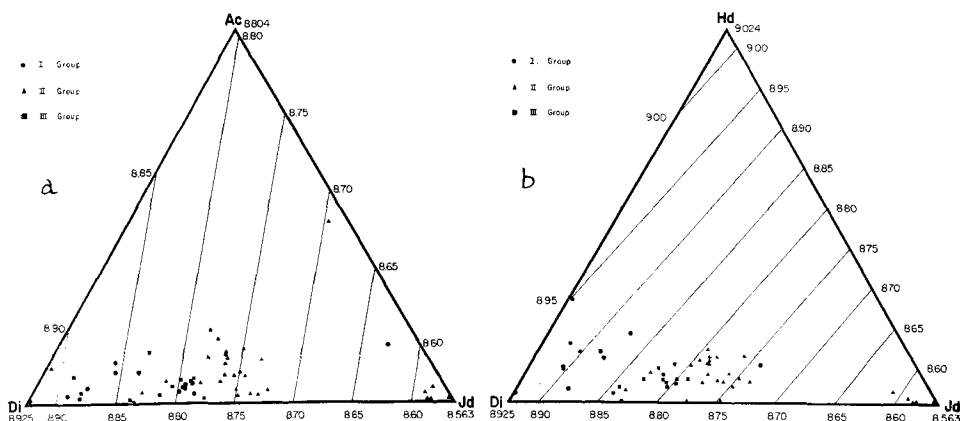


FIG. 2: *a*, Pyroxenes plotted in the system Ac–Di–Jd. *b*, Pyroxenes plotted in the system Hd–Di–Jd.

observed parameters. However, because of the similarities in the orientation of the isoparameter lines these diagrams are of little use in determining compositions of the pyroxenes.

In an attempt to correlate more closely the cell parameters and compositions of these pyroxenes, each composition has been projected from the acmite and hedenbergite apices on to the diopside–jadeite join by producing a line from the apex through the plotted composition (figs. 2 *a* and *b*) to cut the join. This method of projection is believed to be better than merely producing a perpendicular line from the pyroxene composition to the diopside–jadeite join as this gives no indication of the proportion of either acmite or hedenbergite in the bulk composition. Results of this projection are shown in figs. 3 *a* and *b* in which the observed *b* parameter is plotted against the ‘projected’ composition. With very few exceptions, there is, to a first approximation, a linear relationship between the *b* parameter and composition, with in most cases the deviation being small from the expected parameter, drawn between the *b* parameter of pure diopside and pure jadeite (straight line on figs. 3 *a* and *b*). Contrary to the suggestion of Seki and Onuki (1967) there is no evidence of significant curvature in these plots. Nor is there any evidence that the miscibility gap in the diopside–jadeite series does not exist in natural pyroxenes.

In cases where the deviation is large (samples 42, 54, 55) the discrepancies can be accounted for by the samples containing large amounts of acmite, hedenbergite, or Tschermak's molecules, by lack of confidence in the chemical analysis, or more rarely by lack of confidence in the cell parameters.

By measuring the b parameter and comparing it with the theoretical b parameter for diopside-jadeite solid solutions it is possible to determine to within ± 5 mol % the diopside-jadeite ratio of most of the pyroxenes, which, as discussed below, is important to an understanding of the genesis of eclogitic pyroxenes. Although the errors in

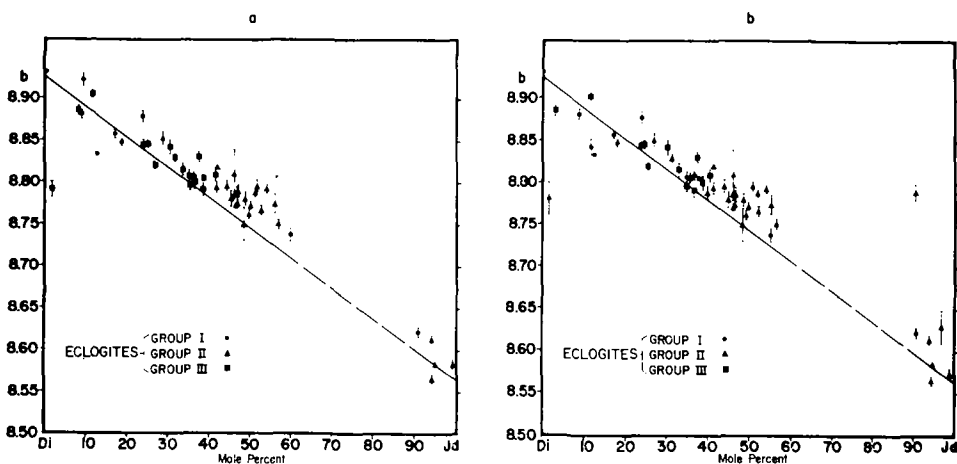


Fig. 3: a , b parameter *v.* mol % Jd by projection from the Ac apex (fig. 2a). Length of bar indicates error. b , parameter *v.* mol % Jd by projection from the Hd apex (fig. 2b). Length of bar indicates error.

the recalculation procedure of this method are small, since over 80 % of the constituents of the samples are used in the recalculation method, large errors are to be expected if the samples contain a high proportion of molecules other than diopside and jadeite. Fortunately, this is rare with omphacitic pyroxenes. Examination of the compositions plotted on the diopside-jadeite-acmite triangle (fig. 2a) and the corresponding projected compositions (fig. 3a) suggests that highly acmitic pyroxenes have b parameters that plot above the theoretical diopside-jadeite line. If sufficient samples had been available it might have been possible to draw further lines in fig. 3a showing the expected parameters for samples with known amounts of acmite. In theory, since the acmite b parameter has an intermediate value to that of diopside and jadeite (table V) such lines should cross the theoretical diopside-jadeite b parameter line. No such relationship is observed with the samples recalculated into diopside-jadeite-hedenbergite molecules.

Because of the method of recalculation of the analysis into either the diopside-jadeite-acmite or diopside-jadeite-hedenbergite molecules, slightly different ratios of diopside to jadeite are obtained depending on which determinative curve of the

projected parameters is used. Fig. 3*b*, showing projection from the hedenbergite apex shows the 'best fit' and therefore probably gives the most accurate diopside-jadeite ratio.

On figs. 3*a* and *b* the samples have been arranged depending on the type of eclogite they occur in. Inspection of these figures shows that the *b* parameters of the omphacites fall into fairly distinct groups. Thus measurement of the *b* parameter of the omphacite proves a rough indicator of the type of eclogite in which it occurs.

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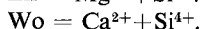
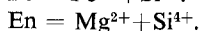
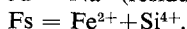
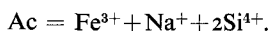
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APPENDIX

Method of recalculation of chemical analysis into the diopside-jadeite-acmite and diopside-jadeite-hedenbergite series of end-member molecules

The method described is a modification of that proposed by Tröger (1962):

From the weight percentage oxides, recalculate cation percentages on the basis of 6·000 oxygen atoms, and from the cation percentages, recalculate into five end-member molecules:



Recalculate these five end-members to 100 %, discarding other cations (principally Al^{3+} , Ti^{4+} , Mn^{2+} , etc.), which will generally be small. The five molecules usually constitute more than 80 % of the available cations and for many samples more than 90 %.

If the analysis is to be recalculated into the diopside-jadeite-acmite molecules proceed:

Ac and Jd are already recalculated.

Form Di by taking equal proportions of Wo and En.

Recalculate the Ac, Jd, Di to 100 %.

Or if the analysis is to be recalculated into the diopside-jadeite-hedenbergite molecules proceed:

Jd is already recalculated.

Form Di by taking equal proportions of Wo and En.

Form Hd by taking equal proportions of residual Wo and Fs.

Recalculate the Jd, Di, Hd to 100 %.